

Locating All Minima of a Smooth Function Without Access to its Derivative

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Motivation

- ▶ We want to identify distinct, “high-quality”, local minimizers of

$$\text{minimize } f(x)$$

$$l \leq x \leq u$$

$$x \in \mathbb{R}^n$$

- ▶ High-quality can be measured by more than the objective.



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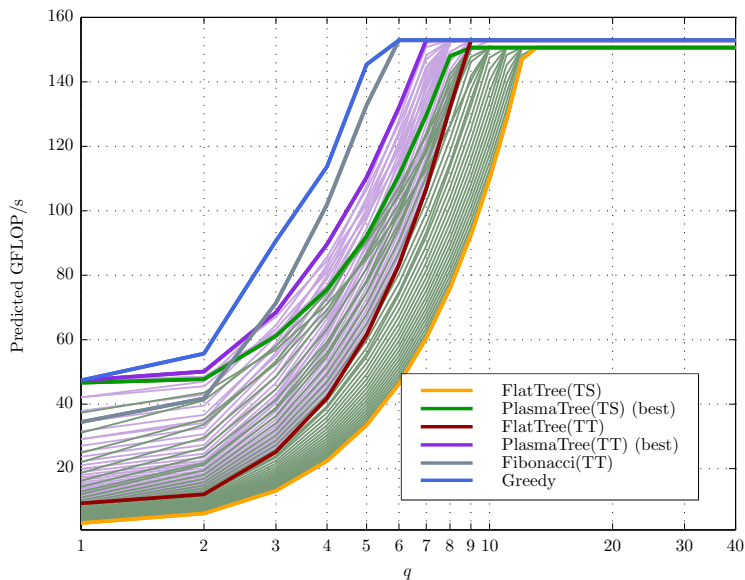
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- ▶ High-quality can be measured by more than the objective.
- ▶ Derivatives of f may or may not be available.
- ▶ The simulation f is likely using parallel resources, but it does not utilize the entire machine.



Why concurrency? Tiled QR example



[Bouwmeester, et al., Tiled QR Factorization Algorithms, 2011]



Global optimization is difficult

Theorem (Törn and Žilinskas, *Global Optimization*, 1989)

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The theory can be more than merely checking that a method generates iterates which are dense in the domain.



Multistart Methods

Given some local optimization routine \mathcal{L} :

Algorithm 1: General Multistart

for $k = 1, 2, \dots$ **do**

 Evaluate f at N points drawn from \mathcal{D}

 Start \mathcal{L} at some set (possibly empty) of previously evaluated points



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- ▶ Which points should start runs?
- ▶ If resources are limited, how should points from each run receive priority?
- ▶ Ideally, only one run is started for each minima.
- ▶ Exploring by sampling. Refining with \mathcal{L} .



Multi-Level Single Linkage

Given some local optimization routine \mathcal{L} :

Algorithm 2: MLSL

for $k = 1, 2, \dots$ **do**

 Sample f at N random points drawn uniformly from \mathcal{D}

 Start \mathcal{L} at any sample point x :

- ▶ that has yet to start a run
 - ▶ $\nexists x_i : \|x - x_i\| \leq r_k$ and $f(x_i) < f(x)$
-

[Rinnooy Kan and Timmer, *Mathematical Programming*, 39(1):57–78, 1987]



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Algorithm 2: MLSL

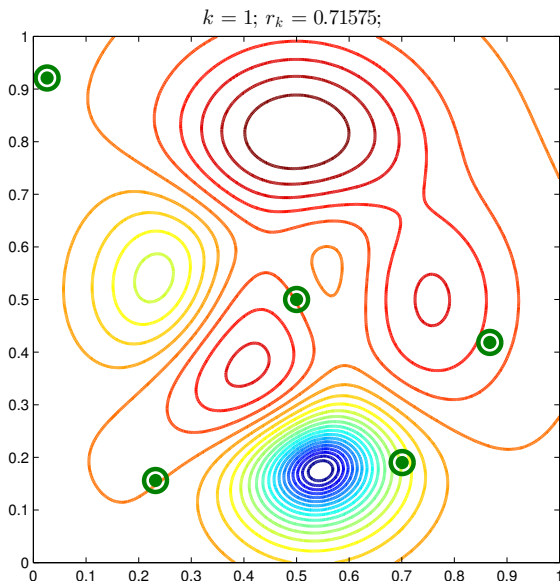
```
for  $k = 1, 2, \dots$  do
    Sample  $f$  at  $N$  random points drawn uniformly from  $\mathcal{D}$ 
    Start  $\mathcal{L}$  at any sample point  $x$ :
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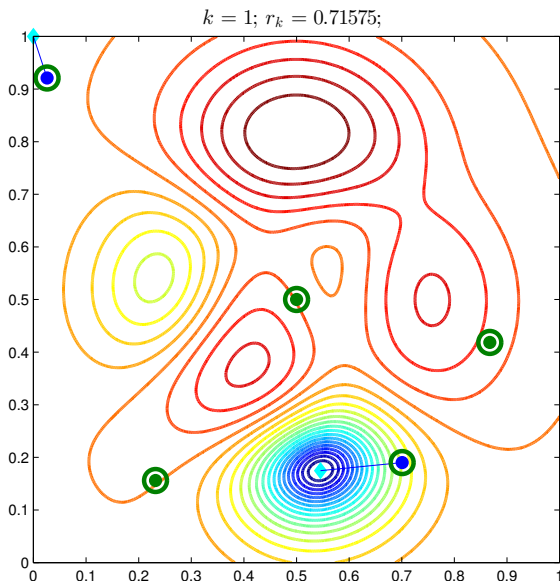
- ▶ Doesn't naturally translate when evaluations of f are limited
- ▶ Ignores some points when deciding where to start \mathcal{L}



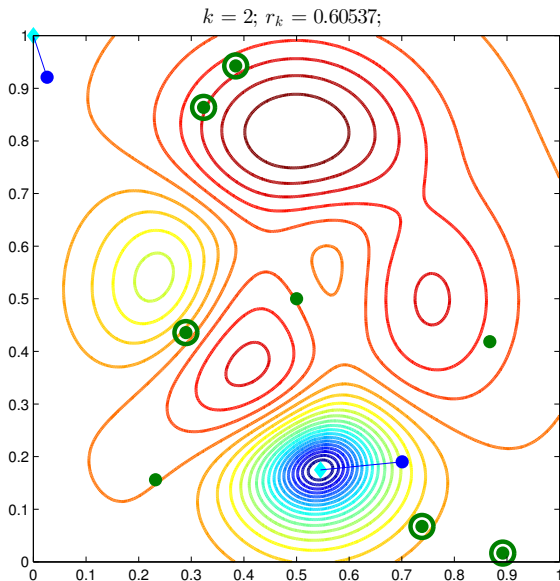
Multi-Level Single Linkage



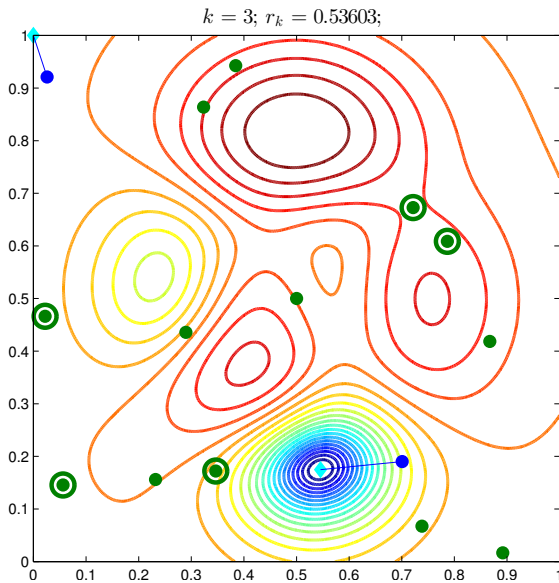
Multi-Level Single Linkage



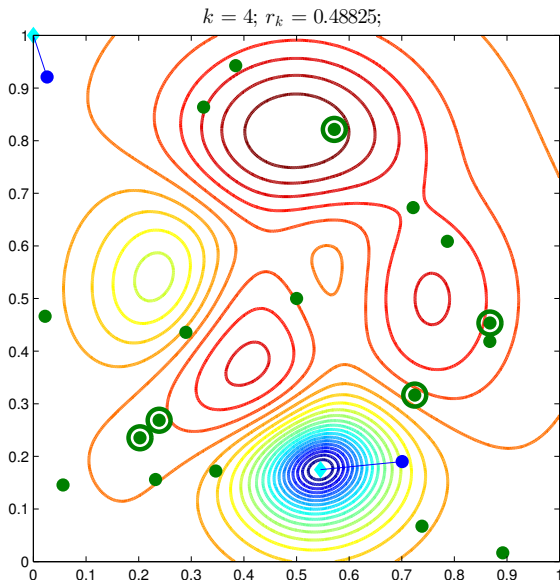
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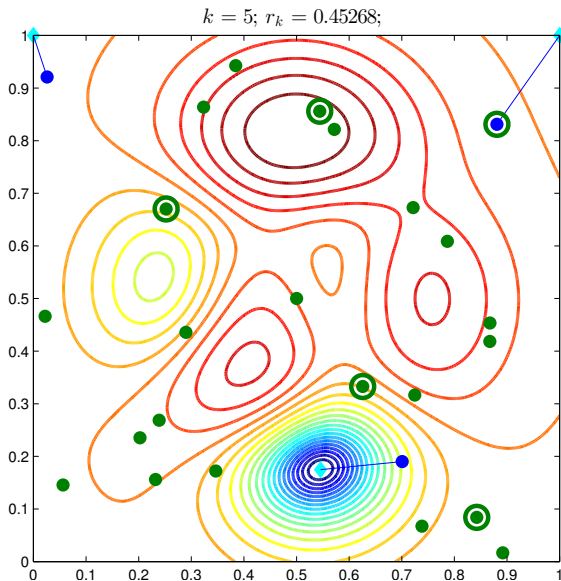
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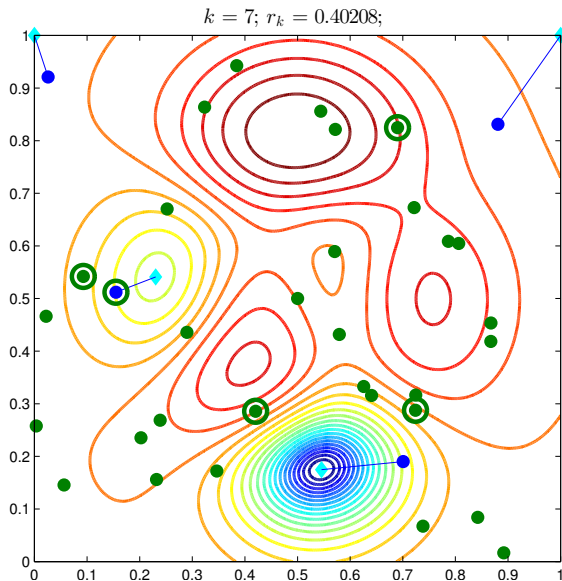
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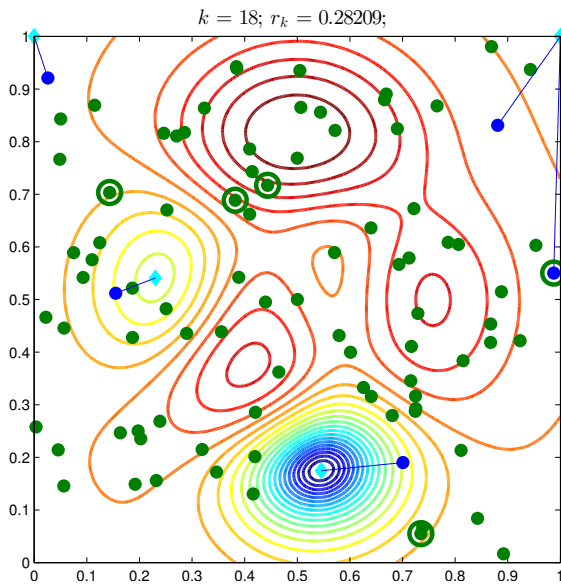
Multi-Level Single Linkage



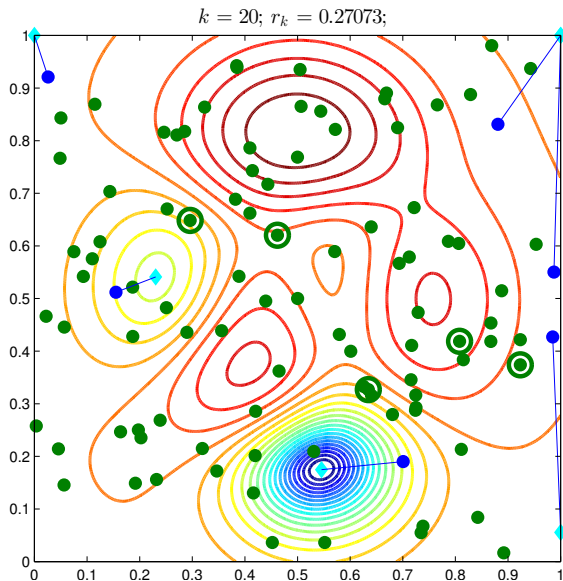
Multi-Level Single Linkage



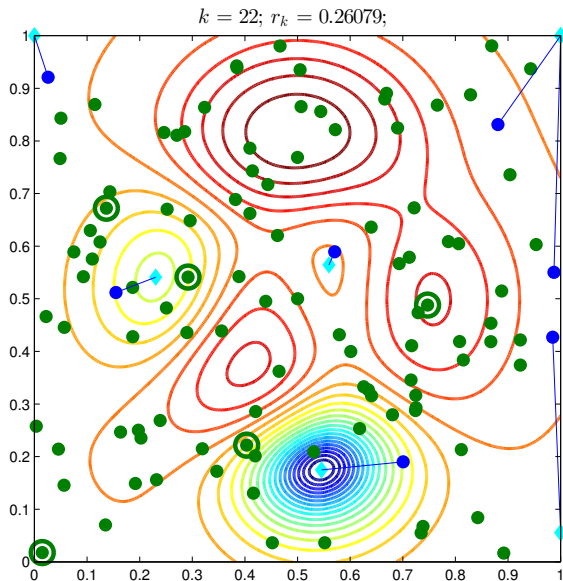
Multi-Level Single Linkage



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Multi-Level Single Linkage

- ▶ $f \in C^2$, with local minima in the interior of \mathcal{D} , and the distance between these minima is bounded away from zero.
- ▶ \mathcal{L} is strictly descent and converges to a minimum (not a stationary point).

▶

$$r_k = \frac{1}{\sqrt{\pi}} \sqrt[n]{\Gamma\left(1 + \frac{n}{2}\right) \text{vol}(\mathcal{D}) \frac{\sigma \log kN}{kN}} \quad (1)$$

Theorem

If $r_k \rightarrow 0$, all local minima will be found almost surely.



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If $r_k \rightarrow 0$, all local minima will be found almost surely.

If r_k is defined by (1) with $\sigma > 4$, even if the sampling continues forever, the total number of local searches started is finite almost surely.



BAMLM

MLSL: (S2)–(S4)

$$\hat{x} \in \mathcal{S}_k$$

- (S2) $\nexists x \in \mathcal{S}_k$ *with*
[$\|\hat{x} - x\| \leq r_k$ *and* $f(x) < f(\hat{x})$]
- (S3) \hat{x} *has not started a local optimization run*
- (S4) \hat{x} *is at least μ from $\partial\mathcal{D}$ and ν from known local minima*



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- (S1) $\nexists x \in \mathcal{L}_k$ with
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- (S2) $\nexists x \in \mathcal{S}_k$ with
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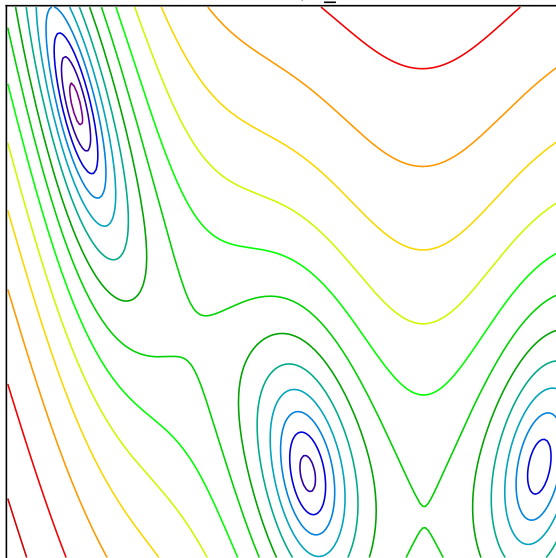
BAMLM: (S1)–(S4), (L1)–(L6)

$$\hat{x} \in \mathcal{L}_k$$

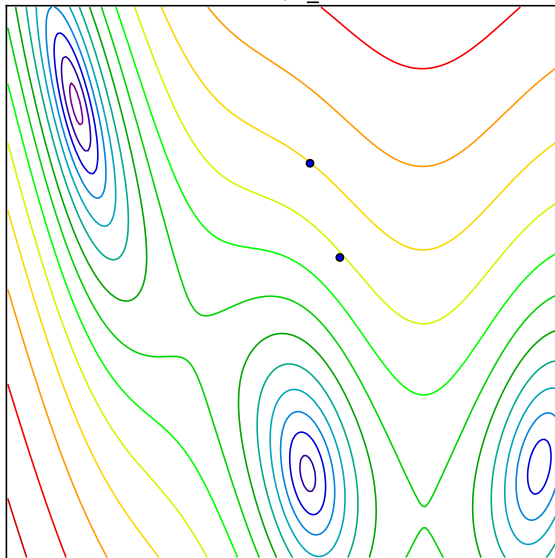
- (L1) $\nexists x \in \mathcal{L}_k$
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- (L3) \hat{x} has not started a local
optimization run
- (L4) \hat{x} is at least μ from $\partial\mathcal{D}$ and ν
from known local minima
- (L5) \hat{x} is not in an active local
optimization run and has not
been ruled stationary
- (L6) $\exists r_k$ -descent path in \mathcal{H}_k from
some $x \in \mathcal{S}_k$ satisfying (S2-S4)
to \hat{x}



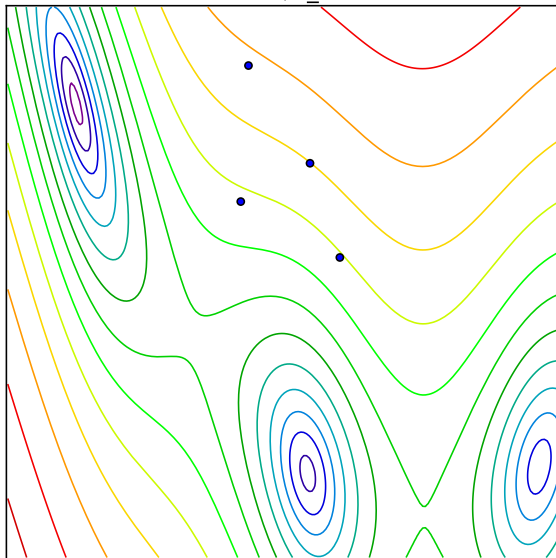
Iteration: 0; r_k : Inf



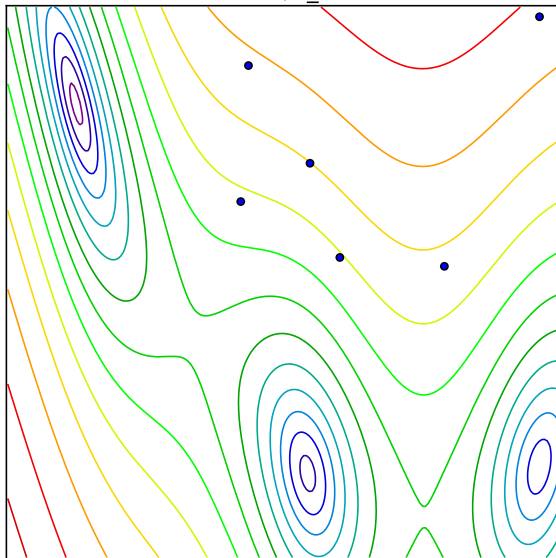
Iteration: 1; r_k : 0.743



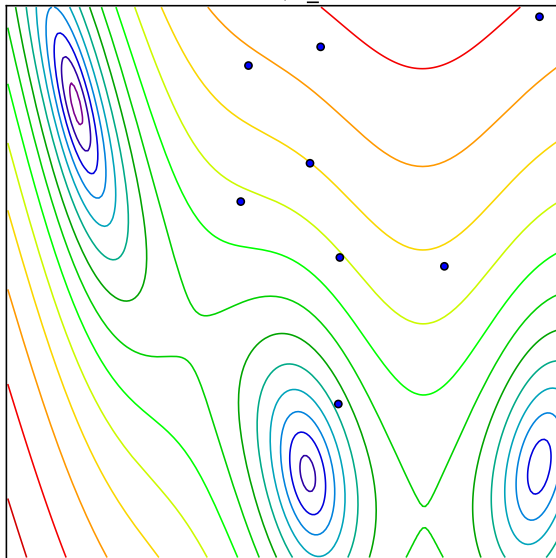
Iteration: 2; r_k : 0.743



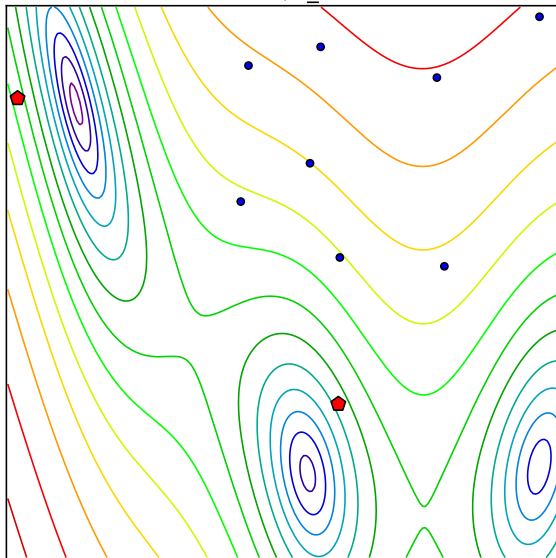
Iteration: 3; r_k : 0.689



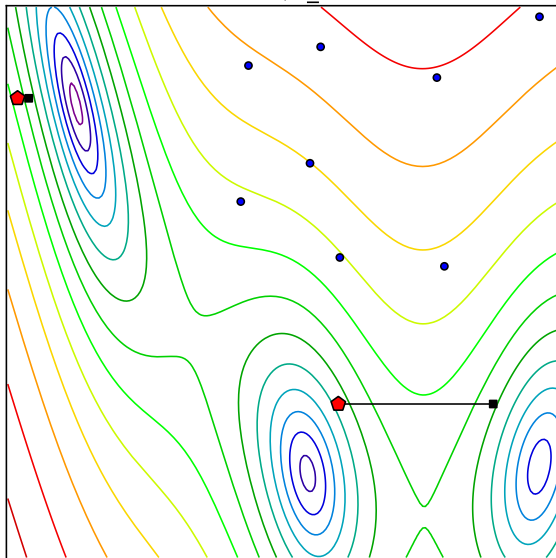
Iteration: 4; r_k : 0.643



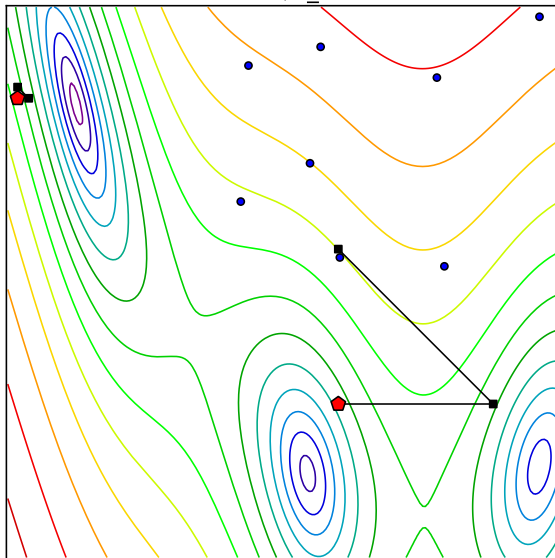
Iteration: 5; r_k : 0.605



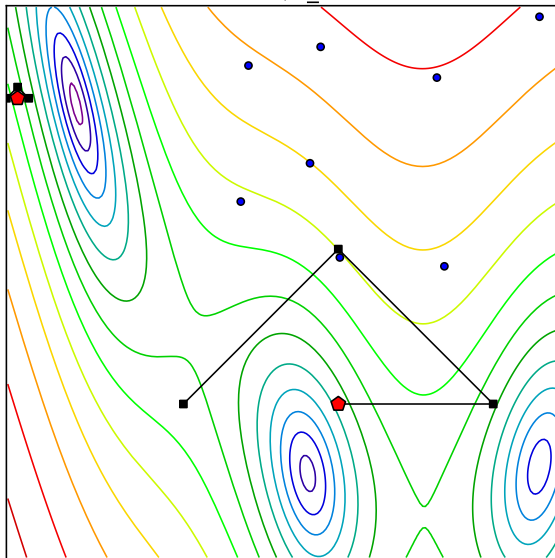
Iteration: 6; r_k : 0.605



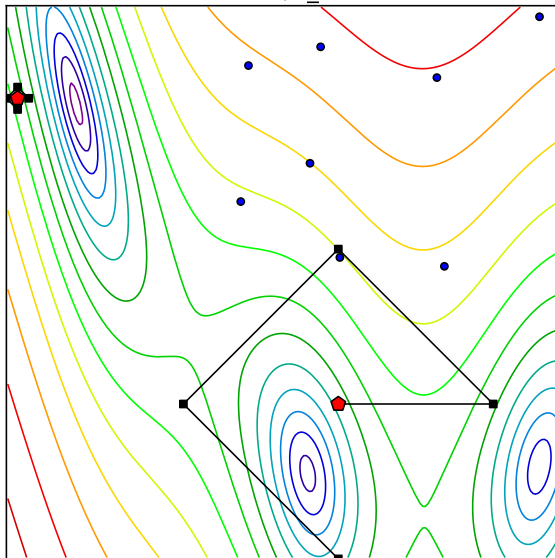
Iteration: 7; r_k : 0.605



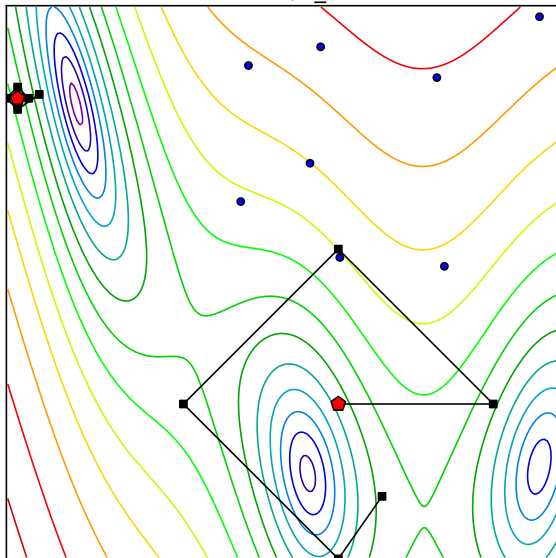
Iteration: 8; r_k : 0.605



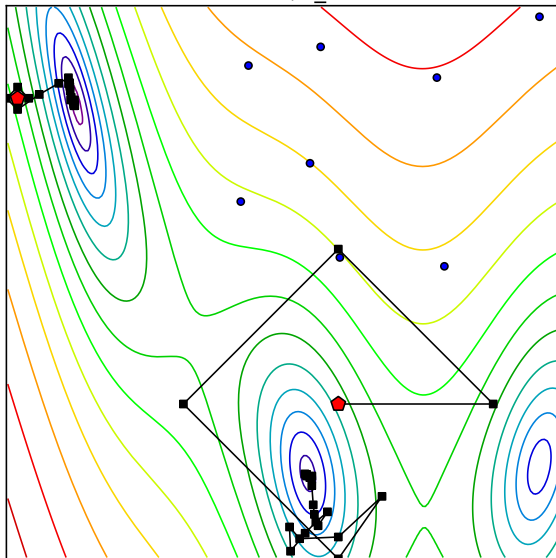
Iteration: 9; r_k : 0.605



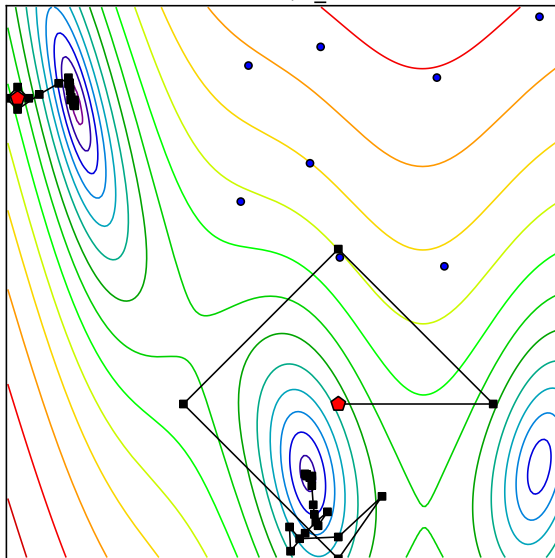
Iteration: 10; r_k : 0.605



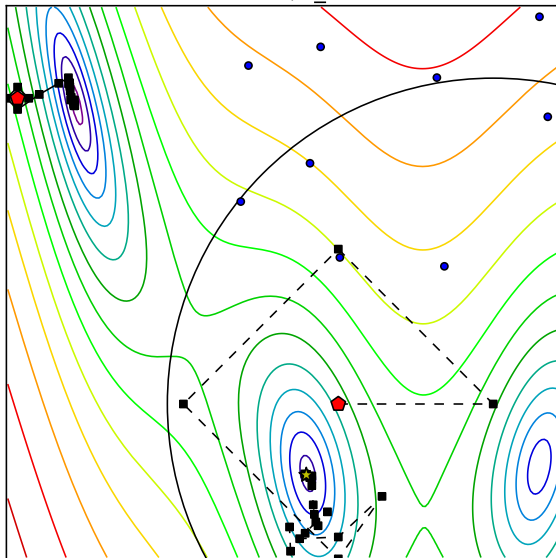
Iteration: 35; r_k : 0.605



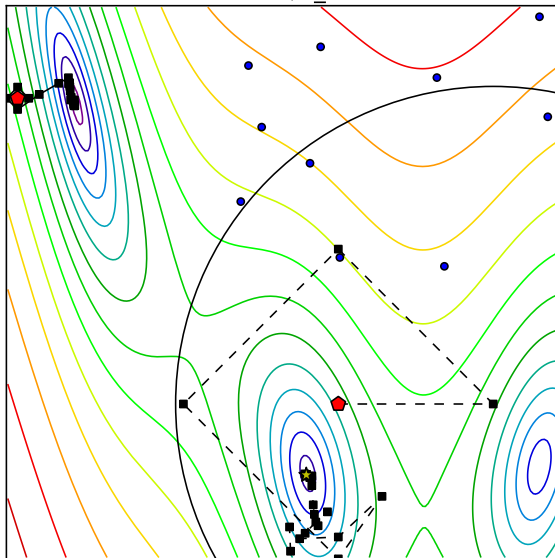
Iteration: 36; r_k : 0.605



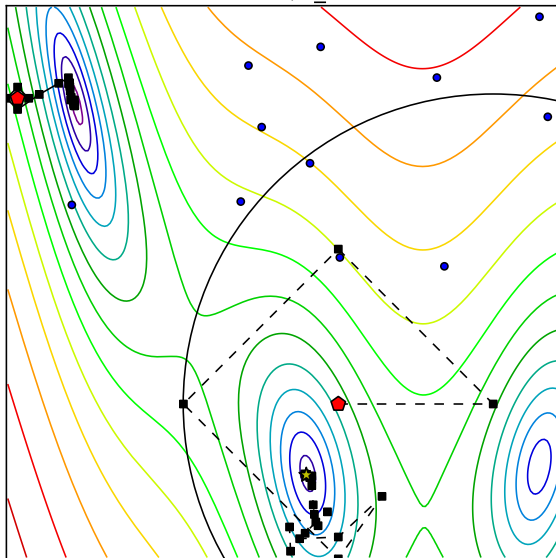
Iteration: 37; r_k : 0.589



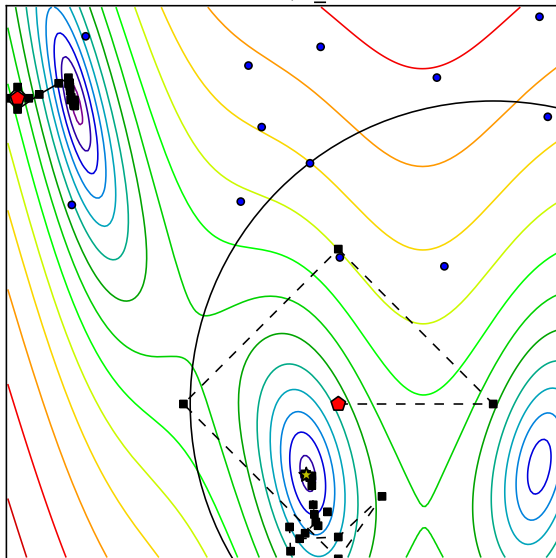
Iteration: 38; r_k : 0.574



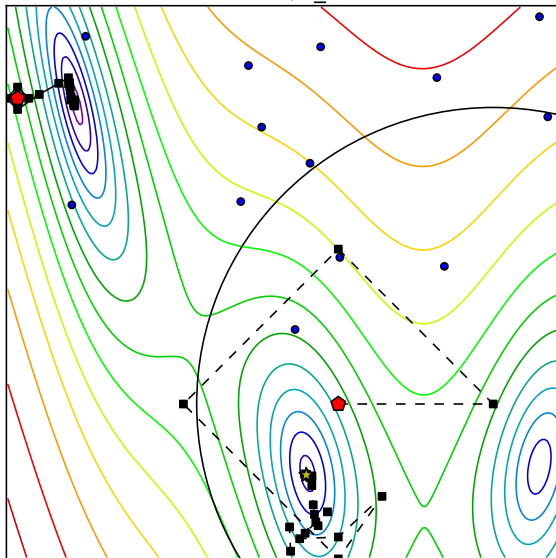
Iteration: 39; r_k : 0.560



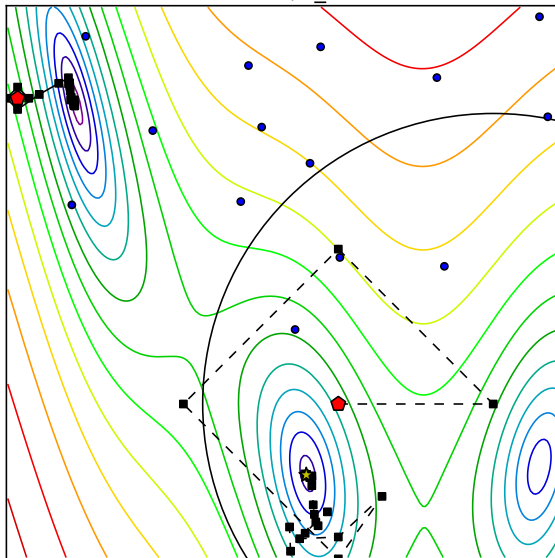
Iteration: 40; r_k : 0.548



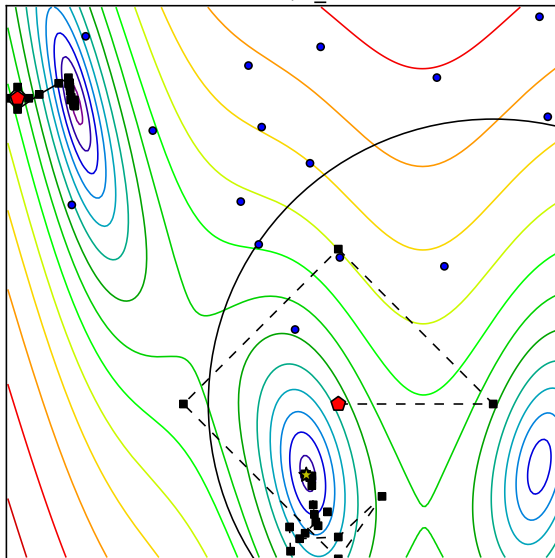
Iteration: 41; r_k : 0.536



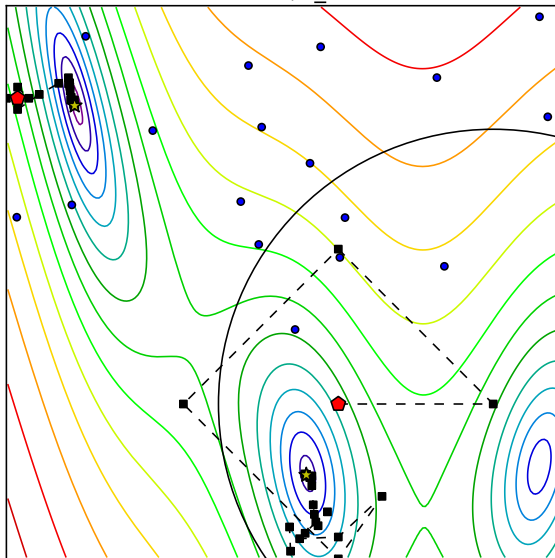
Iteration: 42; r_k : 0.525



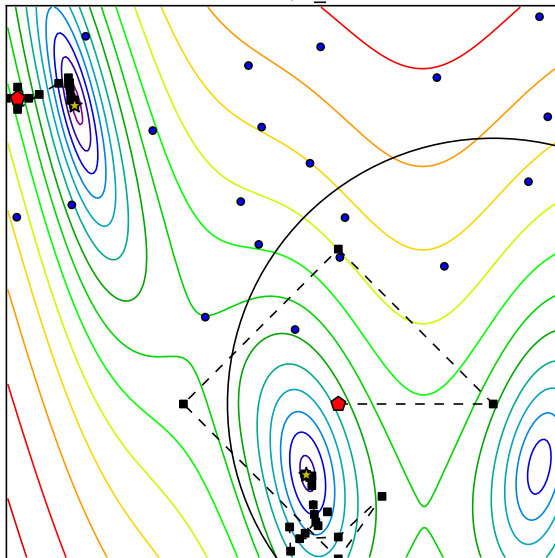
Iteration: 43; r_k : 0.515



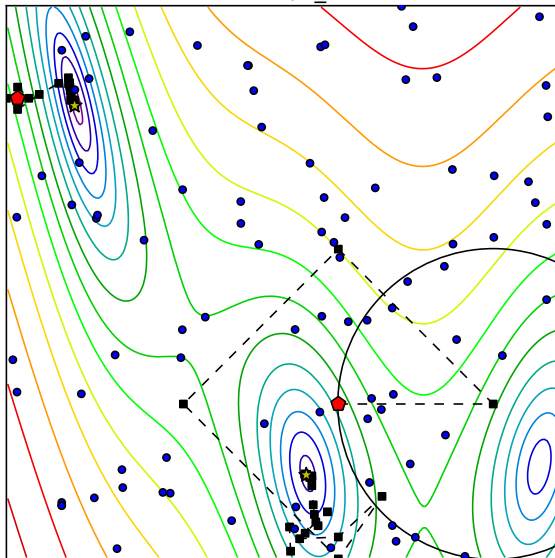
Iteration: 44; r_k : 0.497



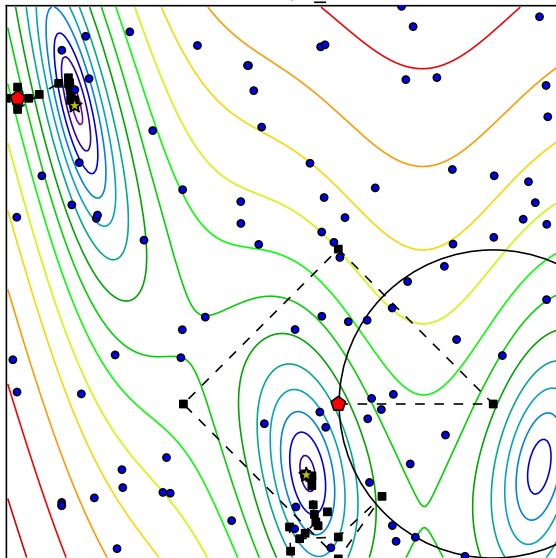
Iteration: 45; r_k : 0.480



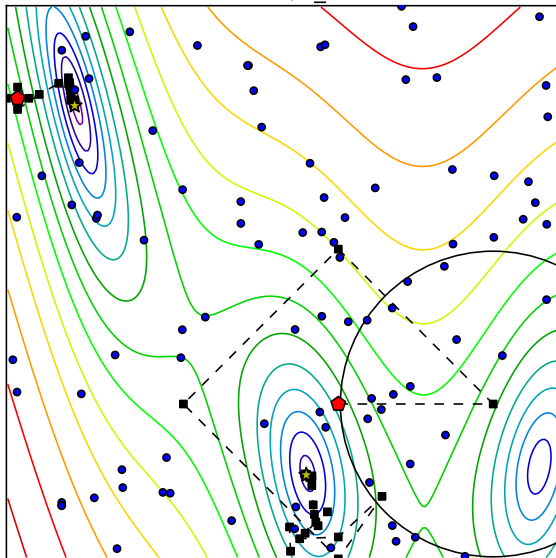
Iteration: 80; r_k : 0.281



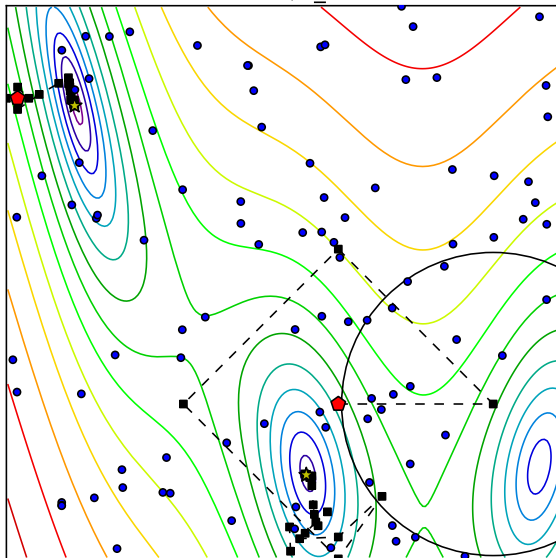
Iteration: 81; r_k : 0.279



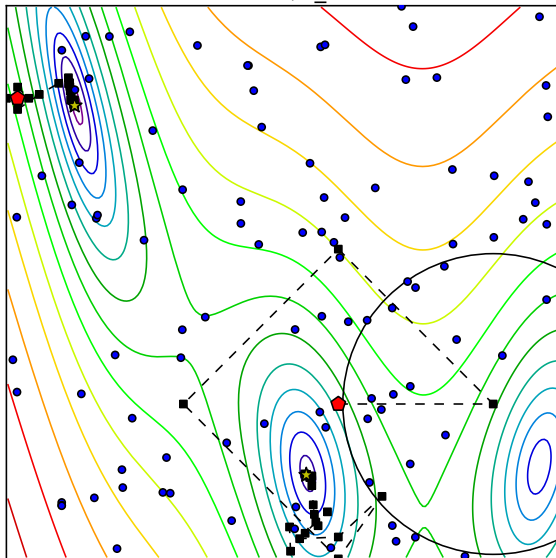
Iteration: 82; r_k : 0.276



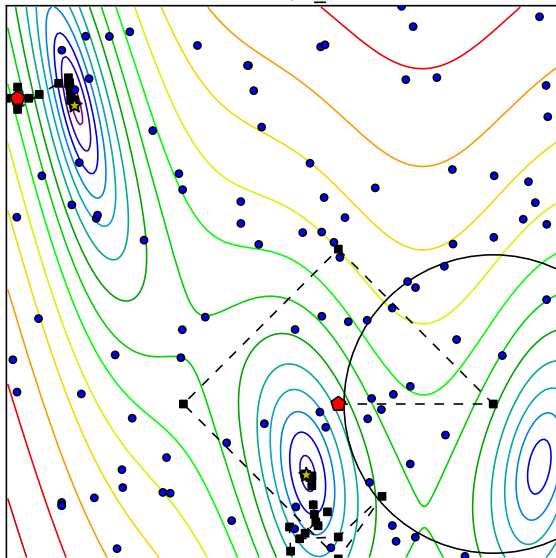
Iteration: 83; r_k : 0.274



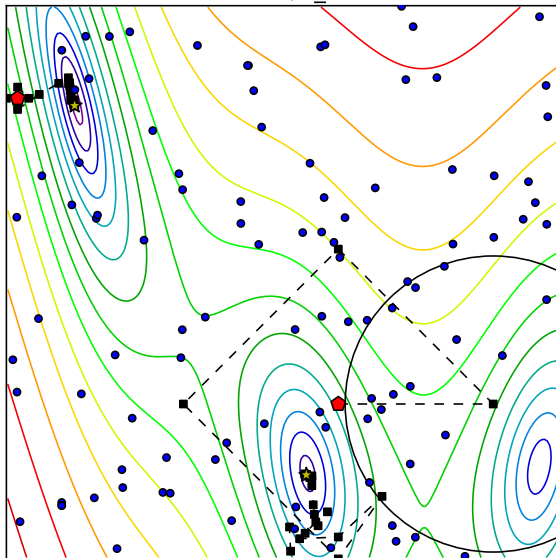
Iteration: 84; r_k : 0.272



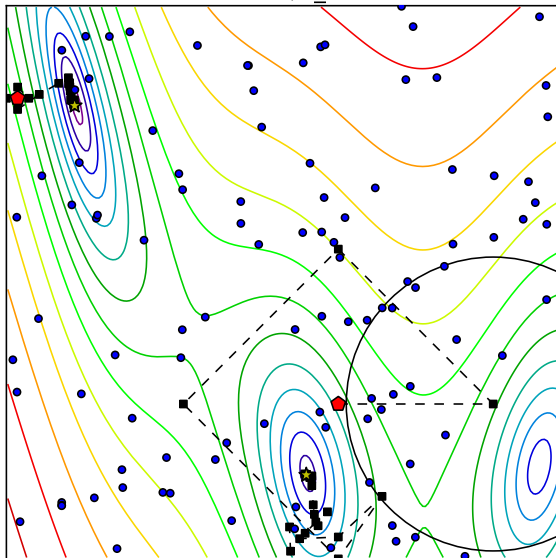
Iteration: 85; r_k : 0.270



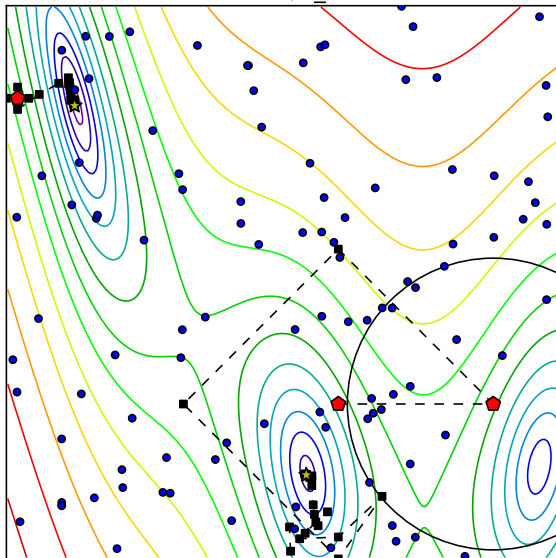
Iteration: 86; r_k : 0.268



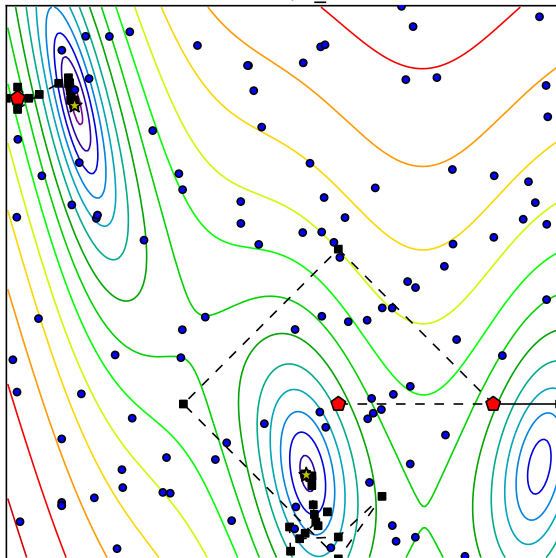
Iteration: 87; r_k : 0.266



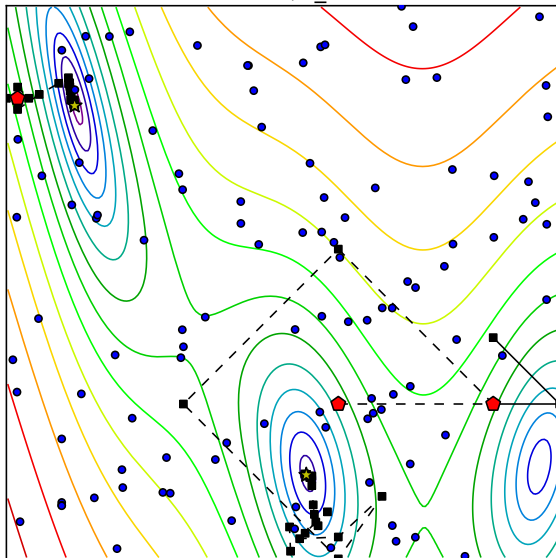
Iteration: 88; r_k : 0.264



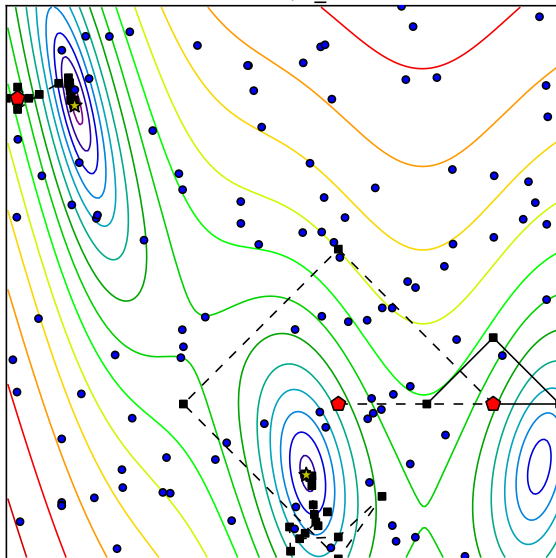
Iteration: 89; r_k : 0.263



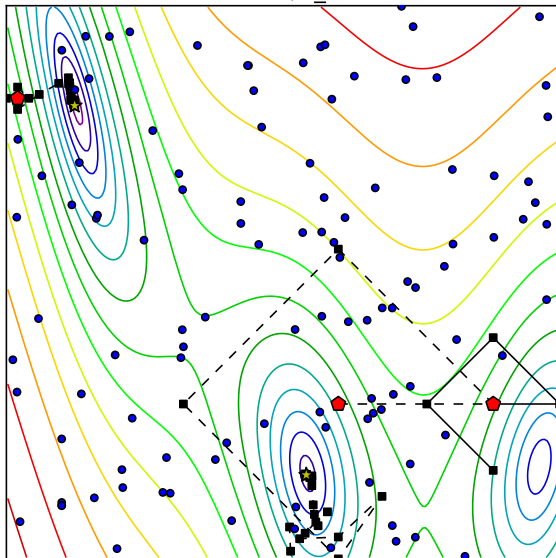
Iteration: 90; r_k : 0.262



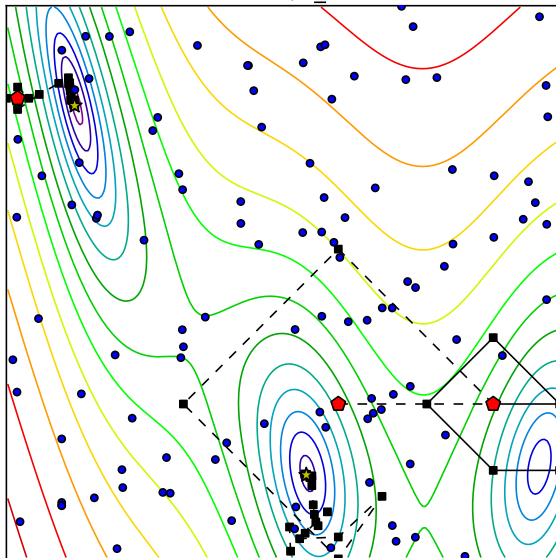
Iteration: 91; r_k : 0.261



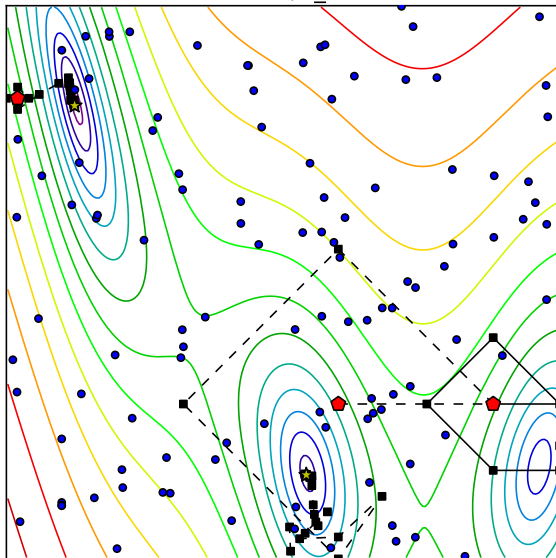
Iteration: 92; r_k : 0.260



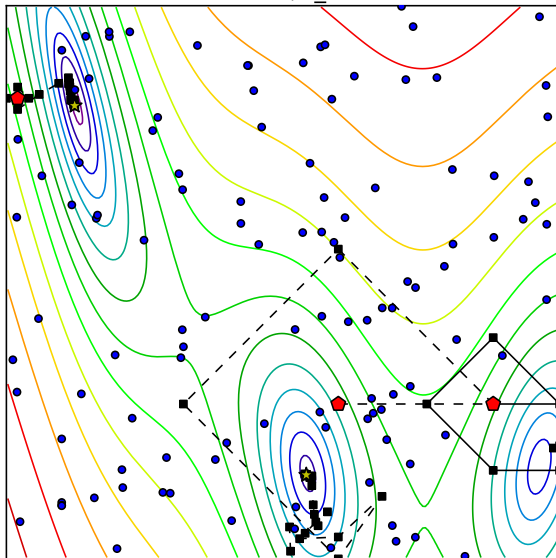
Iteration: 93; r_k : 0.259



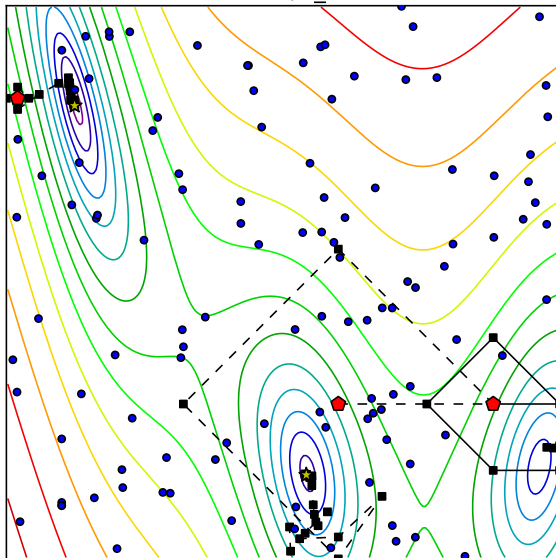
Iteration: 94; r_k : 0.258



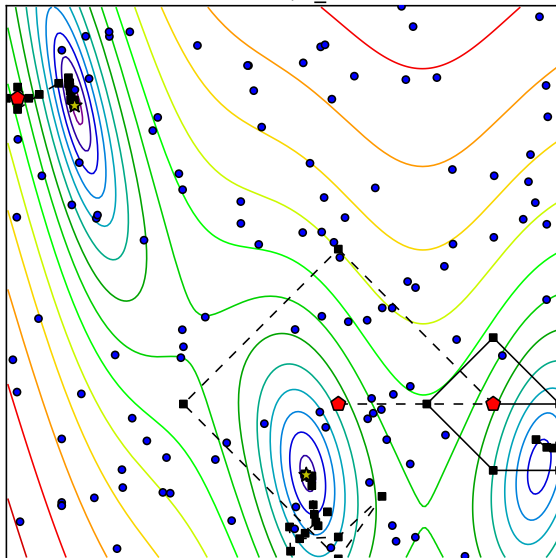
Iteration: 95; r_k : 0.257



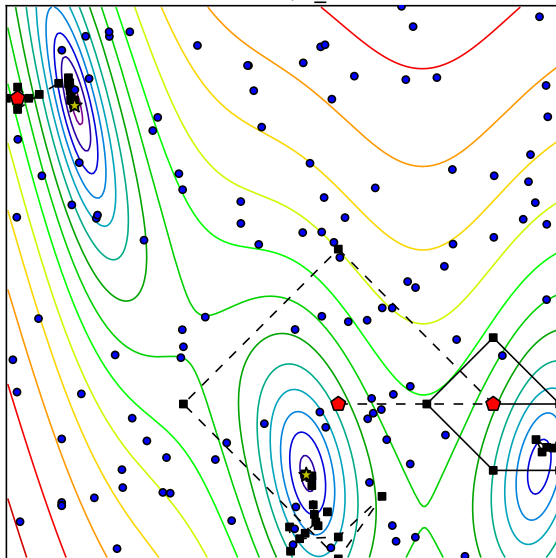
Iteration: 96; r_k : 0.256



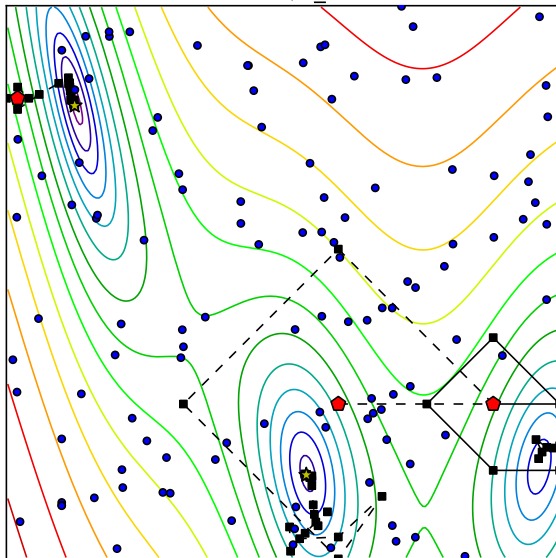
Iteration: 97; r_k : 0.255



Iteration: 98; r_k : 0.255



Iteration: 99; r_k : 0.254



Properties of the local optimization method

Necessary:

- ▶ Honors a starting point
- ▶ Honors bound constraints



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Possibly beneficial:

- ▶ Can return multiple points of interest
- ▶ Reports solution quality/confidence at every iteration
- ▶ Can avoid certain regions in the domain
- ▶ Uses a history of past evaluations of f
- ▶ Uses additional points mid-run



Algorithm 3: AAML

Give each worker a point to evaluate

for $k = 1, 2, \dots$ **do**

 Receive from (longest waiting) worker w that has evaluated f

 Update \mathcal{H}_k and r_k

if *point evaluated by w is from an active run* **then**

if *Run is complete* **then**

 Update X_k^* , and mark points inactive

else

 Add the next point in its localopt run (not in \mathcal{H}_k) to Q_L

 Start run(s) at all point(s) satisfying (S1)–(S4), (L1)–(L6)

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 Merge runs in Q_L with candidate minima within 2ν of each other

 Give w a point at which to evaluate f , either from Q_L or \mathcal{R}

BAMLM

MLSL: (S2)–(S4)

$$\hat{x} \in \mathcal{S}_k$$

- (S1) $\nexists x \in \mathcal{L}_k$ with
[$\|\hat{x} - x\| \leq r_k$ and $f(x) < f(\hat{x})$]
- (S2) $\nexists x \in \mathcal{S}_k$ with
[$\|\hat{x} - x\| \leq r_k$ and $f(x) < f(\hat{x})$]
- (S3) \hat{x} *has not started a local optimization run*
- (S4) \hat{x} *is at least μ from $\partial\mathcal{D}$ and ν from known local minima*

BAMLM: (S1)–(S4), (L1)–(L6)

$$\hat{x} \in \mathcal{L}_k$$

- (L1) $\nexists x \in \mathcal{L}_k$
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[$\|\hat{x} - x\| \leq r_k$ and $f(x) < f(\hat{x})$]
- (L3) \hat{x} has not started a local optimization run
- (L4) \hat{x} is at least μ from $\partial\mathcal{D}$ and ν from known local minima
- (L5) \hat{x} is not in an active local optimization run and has not been ruled stationary
- (L6) $\exists r_k$ -descent path in \mathcal{H}_k from some $x \in \mathcal{S}_k$ satisfying (S2-S4) to \hat{x}



Theorem

Given the same assumptions as MLSL, AAML will start a finite number of local optimization runs with probability 1.



AAML Theory

Theorem

Given the same assumptions as MLSL, AAML will start a finite number of local optimization runs with probability 1.

Assumption

There exists $K_0 < \infty$ so that for any K_0 consecutive iterations, there is a positive (bounded away from zero) probability of evaluating a point from the sample stream and each existing local optimization run.



AAML Theory

Theorem

Given the same assumptions as MLSL, AAML will start a finite number of local optimization runs with probability 1.

Assumption

There exists $K_0 < \infty$ so that for any K_0 consecutive iterations, there is a positive (bounded away from zero) probability of evaluating a point from the sample stream and each existing local optimization run.

Theorem

Each $x^* \in X^*$ will almost surely be either identified in a finite number of evaluations or have a single local optimization run that is converging asymptotically to it.



Measuring Performance

GLODS Global & local optimization using direct search [Custódio, Madeira (JOGO, 2014)]

Direct Serial DIRECT [D. Finkel's MATLAB code]

pVTDirect Parallel DIRECT [He, Watson, Sosonkina (TOMS, 2009)]

Random Uniform sampling over domain (as a baseline)

BAMLM

- ▶ Concurrency: 4
- ▶ Local optimization method
 - ▶ ORBIT [Wild, Regis, & Shoemaker (SIAM JOSC, 2008)]
 - ▶ BOBYQA [Powell, 2009]
- ▶ Initial sample size: $10n$

- ▶ Each method evaluates Direct's $2n + 1$ initial points.



Measuring Performance

Notation:

Let X^* be the set of all local minima of f .

Let $f_{(i)}^*$ be the i th smallest value $\{f(x^*) | x^* \in X^*\}$.

Let $x_{(i)}^*$ be the element of X^* corresponding to the value $f_{(i)}^*$.

The global minimum has been found at a level $\tau > 0$ at batch k if an algorithm it has found a point \hat{x} satisfying:

$$f(\hat{x}) - f_{(1)}^* \leq (1 - \tau) \left(f(x_0) - f_{(1)}^* \right),$$

where x_0 is the starting point for problem p .



Measuring Performance

Notation:

Let X^* be the set of all local minima of f .

Let $f_{(i)}^*$ be the i th smallest value $\{f(x^*) | x^* \in X^*\}$.

Let $x_{(i)}^*$ be the element of X^* corresponding to the value $f_{(i)}^*$.

The j best local minima have been found at a level $\tau > 0$ at batch k if:

$$\left| \left\{ x_{(1)}^*, \dots, x_{(\underline{j}-1)}^* \right\} \cap \left\{ x_{(i)}^* : \exists x \in \mathcal{H}_k \text{ with } \|x - x_{(i)}^*\| \leq r_n(\tau) \right\} \right| = \underline{j} - 1$$

&

$$\left| \left\{ x_{(\underline{j})}^*, \dots, x_{(\bar{j})}^* \right\} \cap \left\{ x_{(i)}^* : \exists x \in \mathcal{H}_k \text{ with } \|x - x_{(i)}^*\| \leq r_n(\tau) \right\} \right| \geq \bar{j} - \underline{j} + 1,$$

where \underline{j} and \bar{j} are the smallest and largest integers such that

$$f_{(\underline{j})}^* = f_{(\bar{j})}^* = f_{(\underline{j})}^* \text{ and where } r_n(\tau) = \sqrt[n]{\frac{\tau \text{vol}(\mathcal{D}) \Gamma(\frac{n}{2} + 1)}{\pi^{n/2}}}.$$



Problems considered

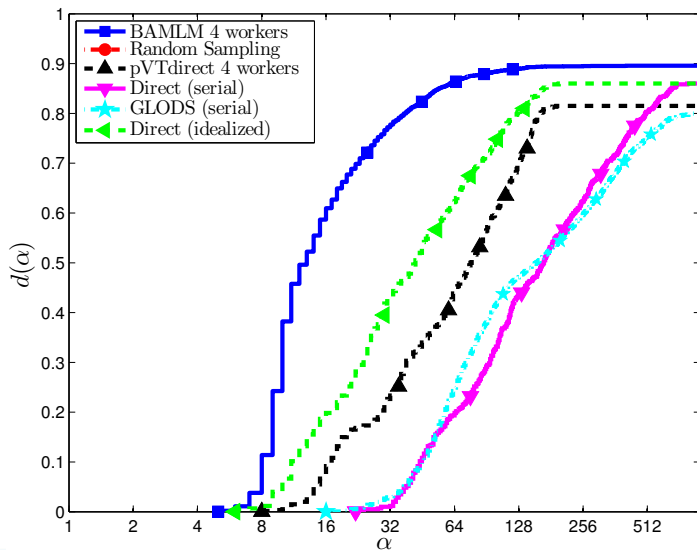
GKLS problem generator [Gaviano et al., “Algorithm 829” (TOMS, 2003)]

- ▶ 600 synthetic problems with known local minima
- ▶ $n = 2, \dots, 7$
- ▶ 10 local minima in the unit cube with a unique global minimum
- ▶ 100 problems for each dimension
- ▶ 5 replications (different seeds) for each problem
- ▶ 5000 evaluations



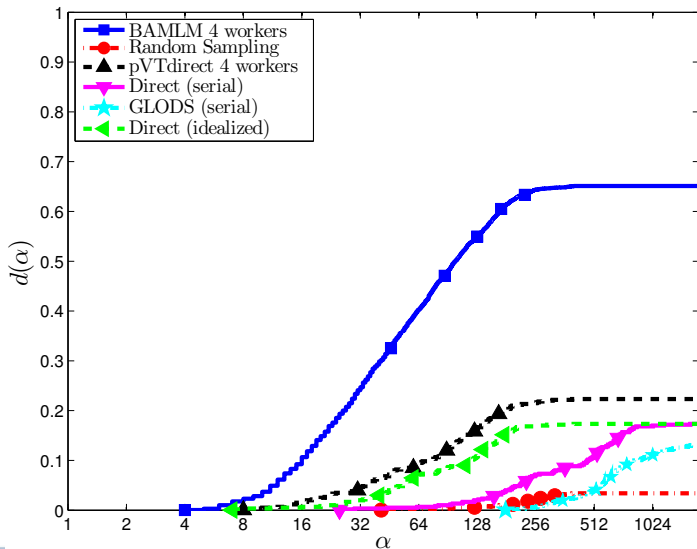
Data Profiles

$$f(x) - f_{(1)}^* \leq (1 - 10^{-5}) \left(f(x_0) - f_{(1)}^* \right)$$



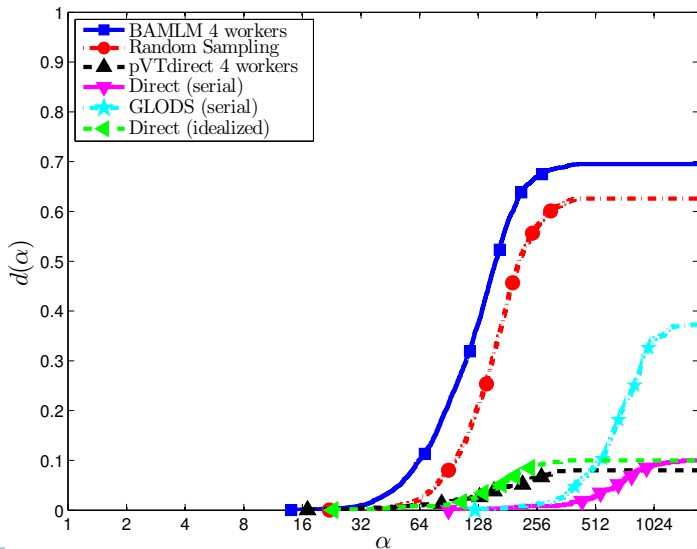
Data Profiles

Within $\sqrt[n]{\frac{10^{-4}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 3 best minima



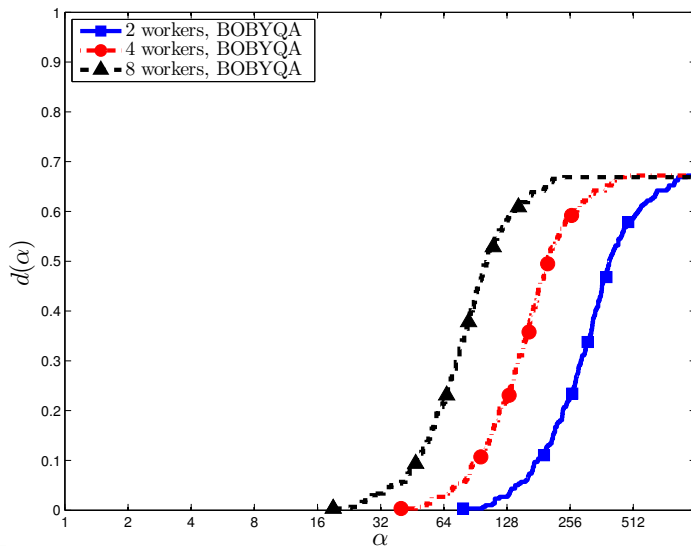
Data Profiles

Within $\sqrt[n]{\frac{10^{-3}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 7 best minima



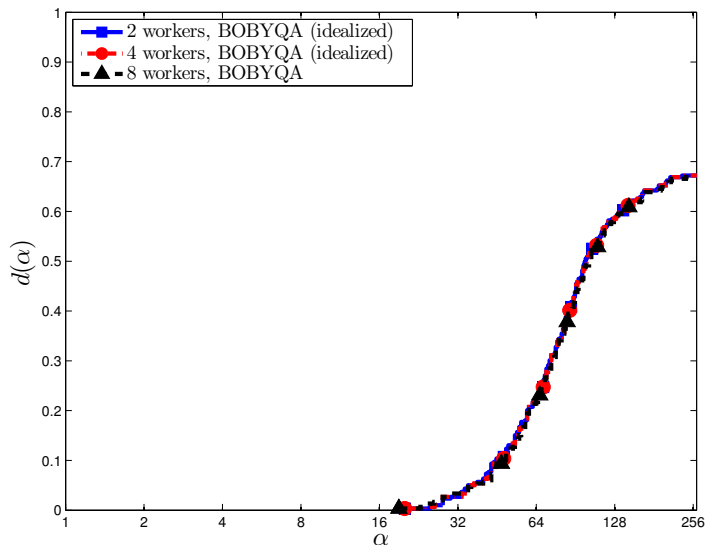
Data Profiles

Within $\sqrt[n]{\frac{10^{-3}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 7 best minima



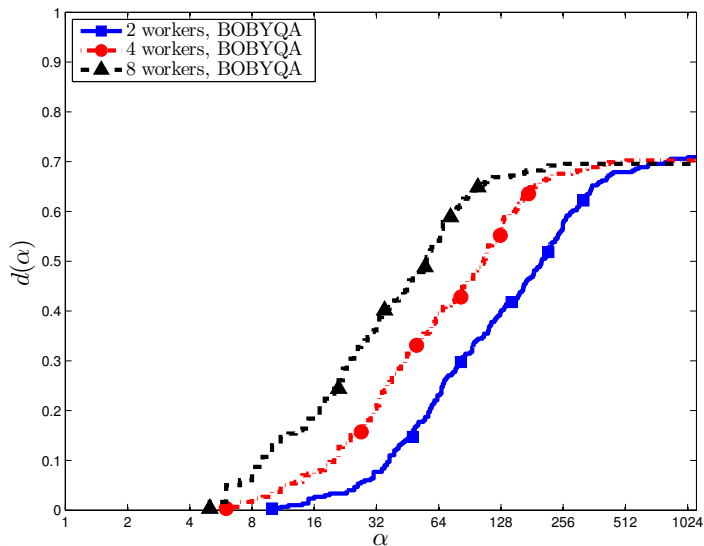
Data Profiles

Within $\sqrt[n]{\frac{10^{-3}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 7 best minima



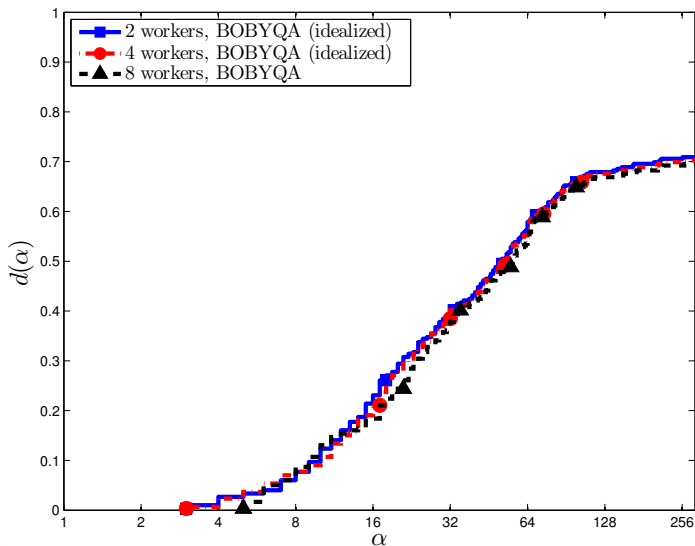
Data Profiles

Within $\sqrt[n]{\frac{10^{-4}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 3 best minima



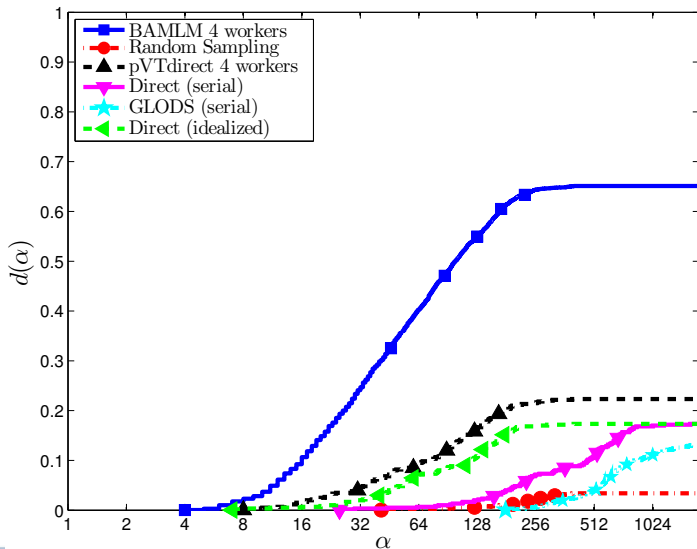
Data Profiles

Within $\sqrt[n]{\frac{10^{-4}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 3 best minima



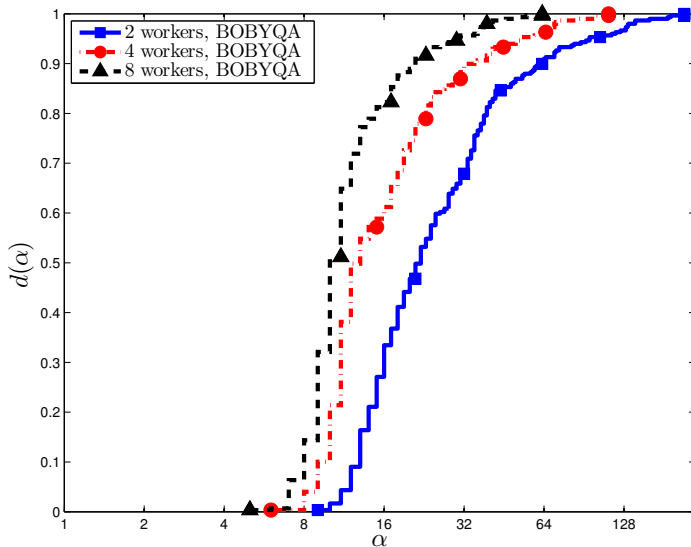
Data Profiles

Within $\sqrt[n]{\frac{10^{-4}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 3 best minima



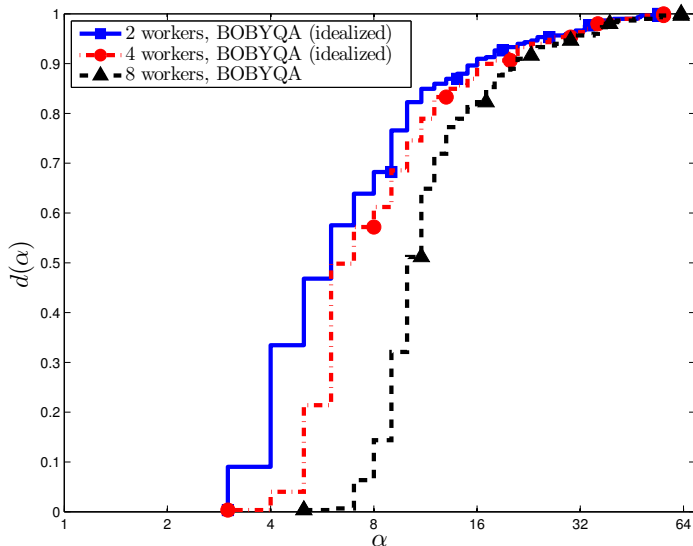
Data Profiles

$$f(x) - f_{(1)}^* \leq (1 - 10^{-5}) \left(f(x_0) - f_{(1)}^* \right)$$

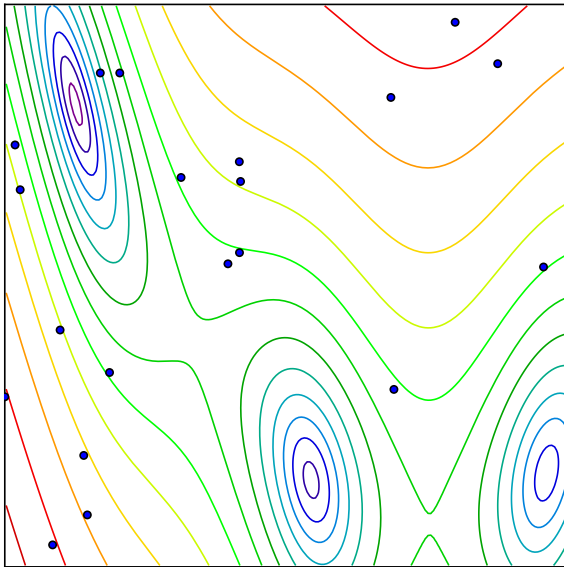


Data Profiles

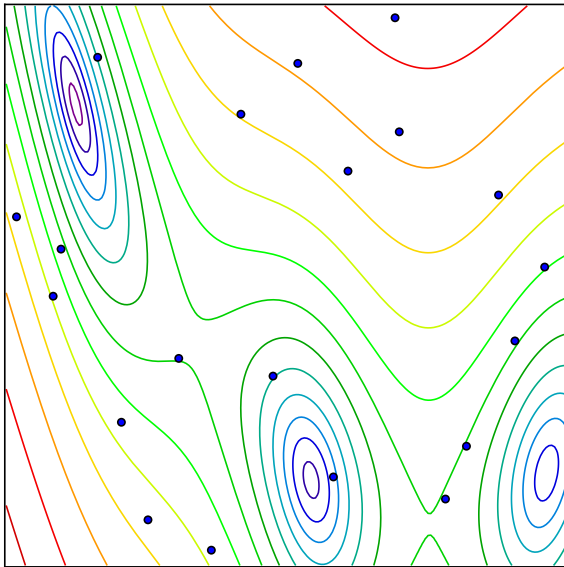
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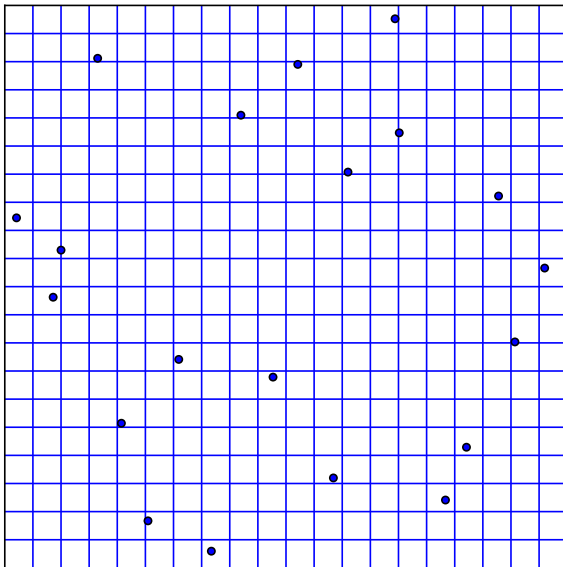
Uniform sampling



Latin hypercube sampling



Latin hypercube sampling



BAMLM with LHS

Critical distance for uniform sampling:

$$r_k = \pi^{-1/2} \left(\Gamma(1 + \frac{n}{2}) \text{vol}(\mathcal{D}) \frac{\sigma \log kN}{kN} \right)^{1/n}$$

Critical distance for Latin hypercube sampling:

$$r_k = \pi^{-1/2} \left(\Gamma(1 + \frac{n}{2}) \text{vol}(\mathcal{D}) \frac{\sigma N^{n-1} \log k}{k} \right)^{1/n} \quad (2)$$



BAMLM with LHS

Critical distance for uniform sampling:

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Critical distance for Latin hypercube sampling:

$$r_k = \pi^{-1/2} \left(\Gamma(1 + \frac{n}{2}) \text{vol}(\mathcal{D}) \frac{\sigma N^{n-1} \log k}{k} \right)^{1/n} \quad (2)$$

Theorem

If r_k is defined by (2) with $\sigma > 4$, even if the sampling continues forever, the total number of local runs started by BAMLM (or AAMLM) is finite almost surely.



Does LHS help?

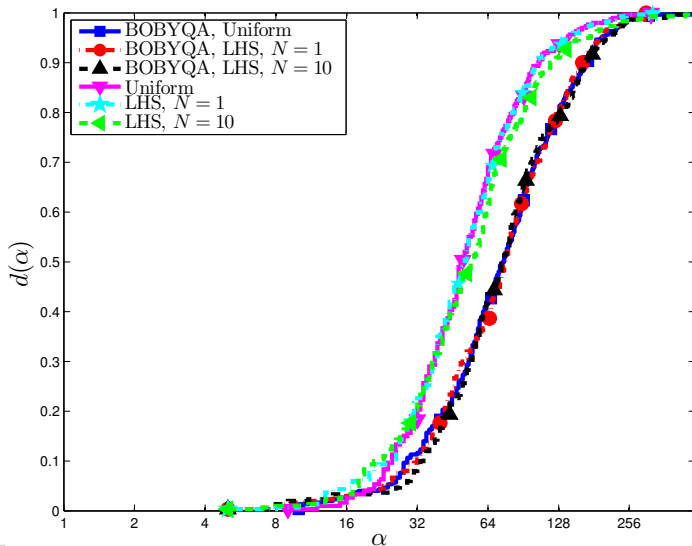
Problem setup:

- ▶ 10 different GKLS problems
- ▶ 5 different seeds
- ▶ $n = 2, \dots, 7$
- ▶ Same starting LHS sample of $10n$ points (except for uniform)
- ▶ Same (uniform) r_k value



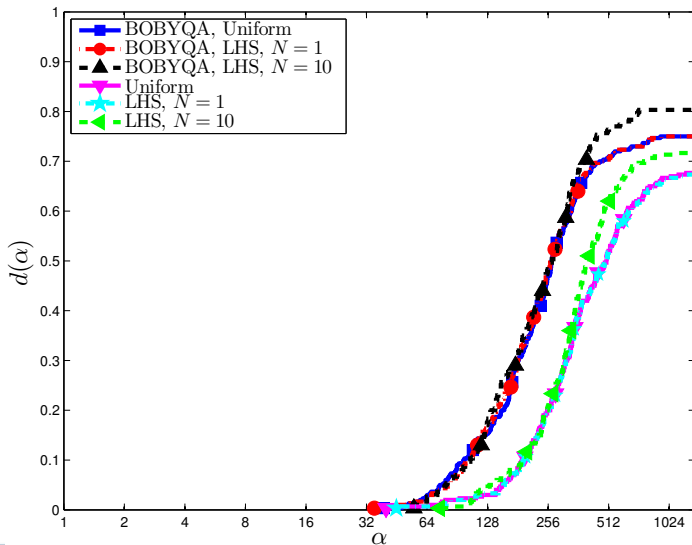
Data Profiles

Within $\sqrt[n]{\frac{10^{-2}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 5 best minima



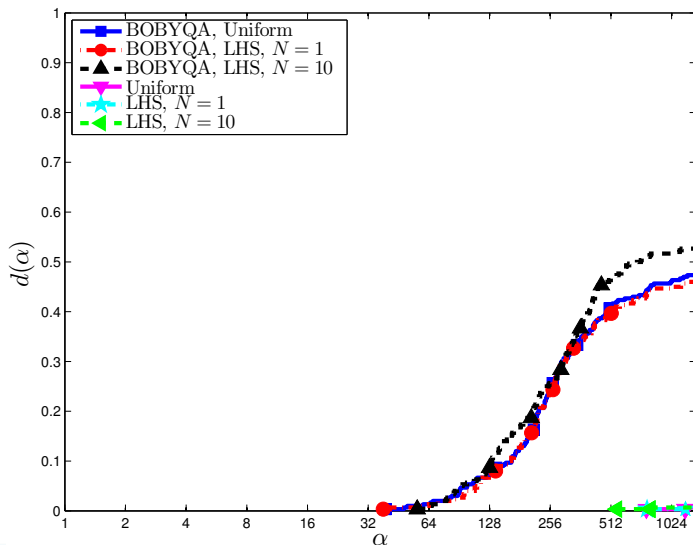
Data Profiles

Within $\sqrt[n]{\frac{10^{-3}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 5 best minima



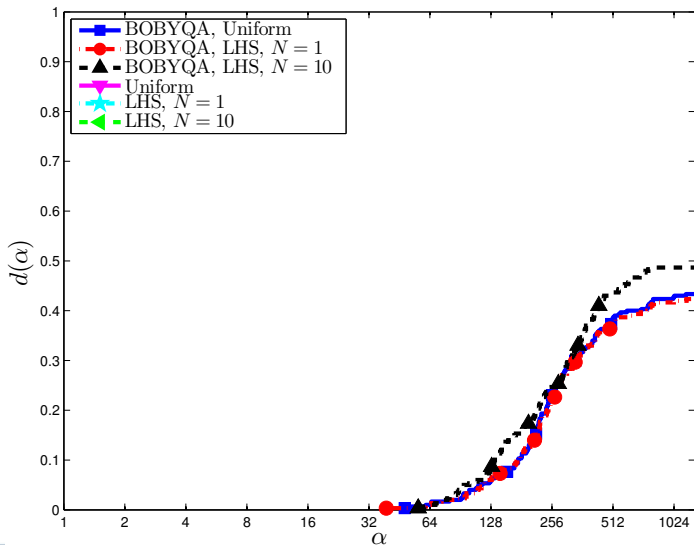
Data Profiles

Within $\sqrt[n]{\frac{10^{-4}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 5 best minima



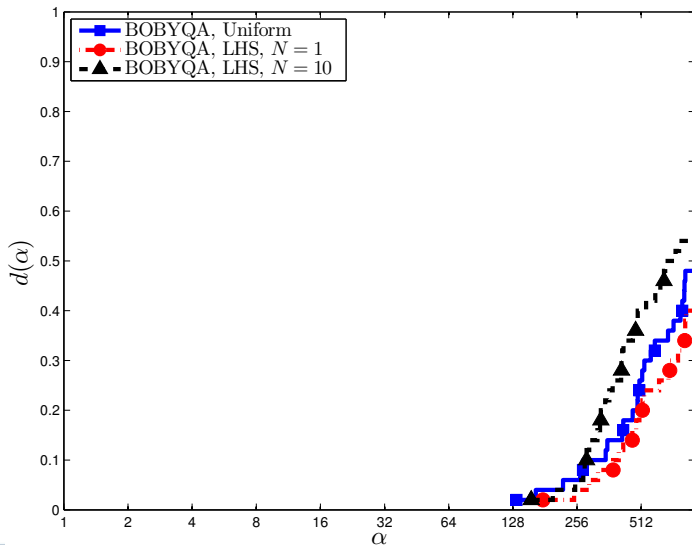
Data Profiles

Within $\sqrt[n]{\frac{10^{-5}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 5 best minima



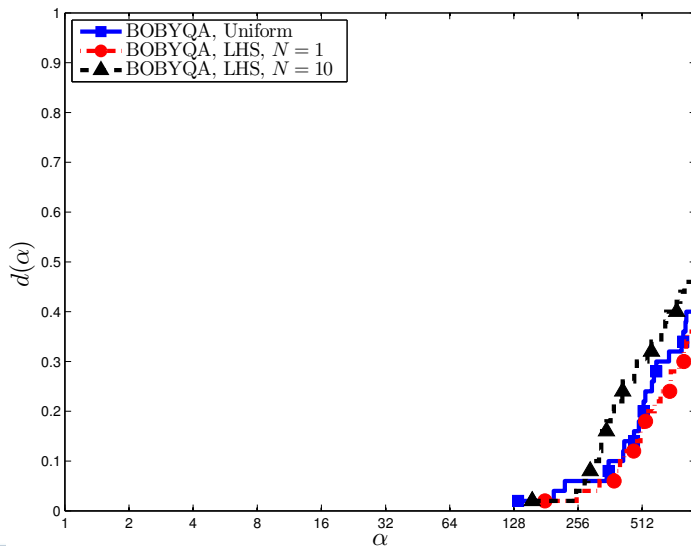
Data Profiles

Within $\sqrt[n]{\frac{10^{-4}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 5 best minima, $n = 6$



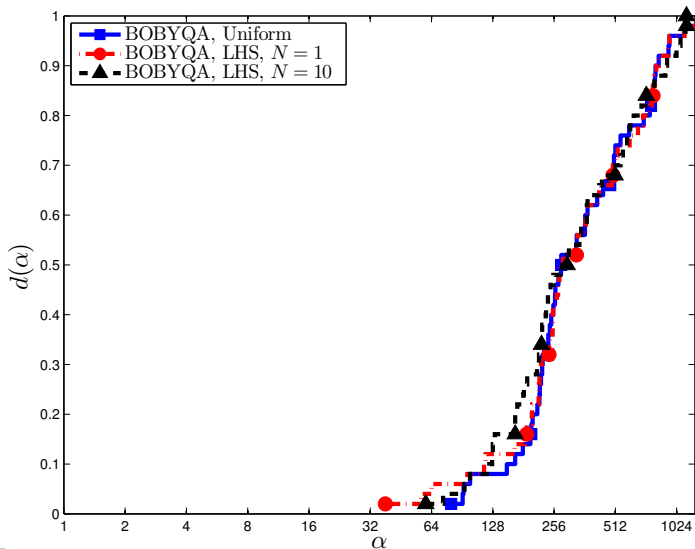
Data Profiles

Within $\sqrt[n]{\frac{10^{-5}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 5 best minima, $n = 6$



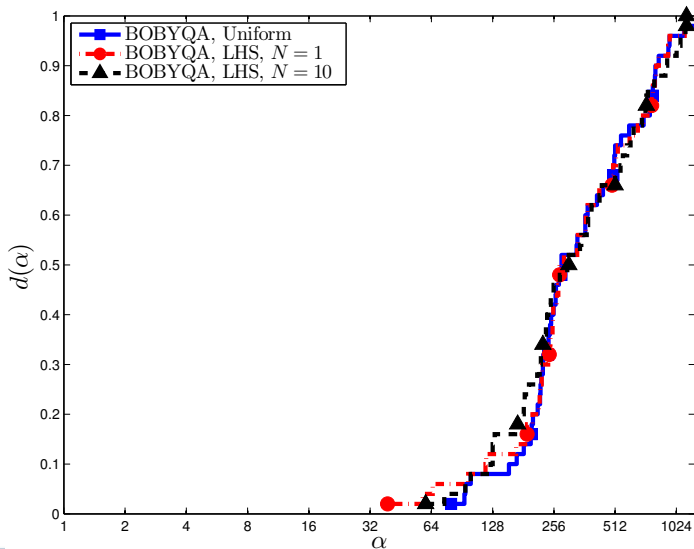
Data Profiles

Within $\sqrt[n]{\frac{10^{-4}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 5 best minima, $n = 3$



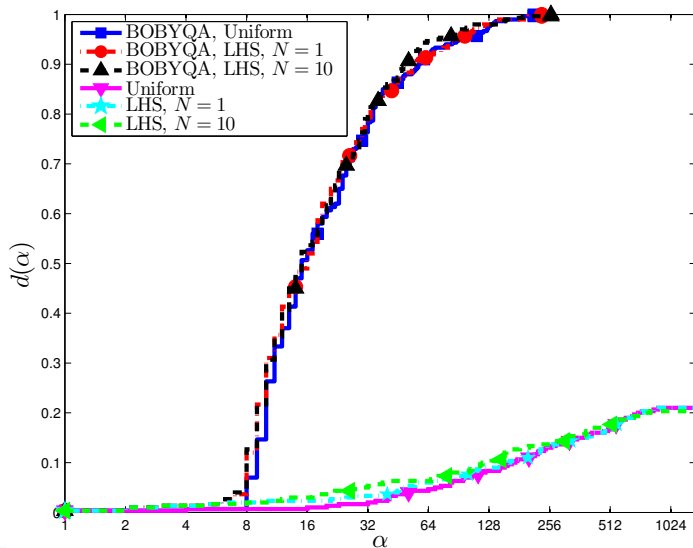
Data Profiles

Within $\sqrt[n]{\frac{10^{-5}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 5 best minima, $n = 3$



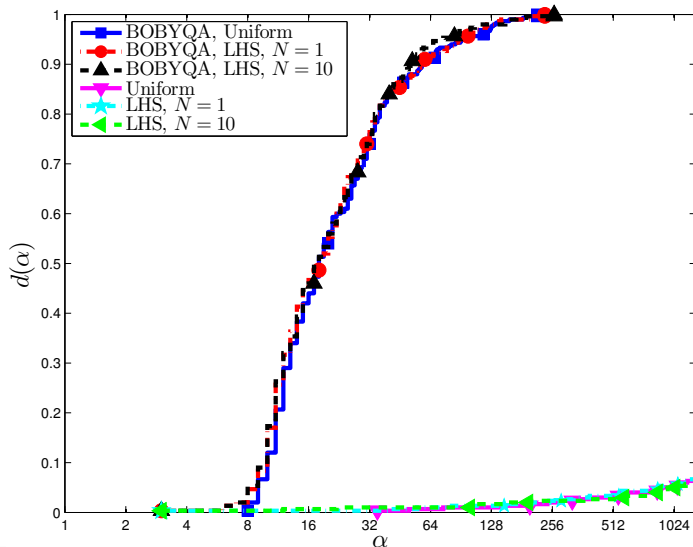
Data Profiles

$$f(x) - f_{(1)}^* \leq (1 - 10^{-2}) \left(f(x_0) - f_{(1)}^* \right)$$



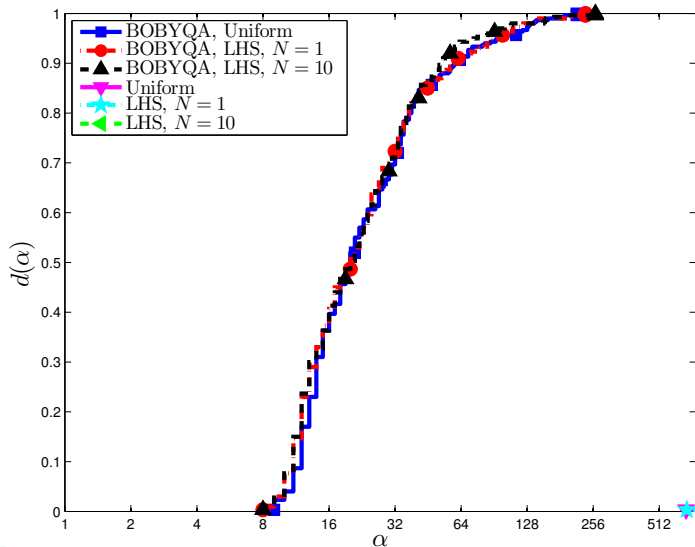
Data Profiles

$$f(x) - f_{(1)}^* \leq (1 - 10^{-3}) \left(f(x_0) - f_{(1)}^* \right)$$



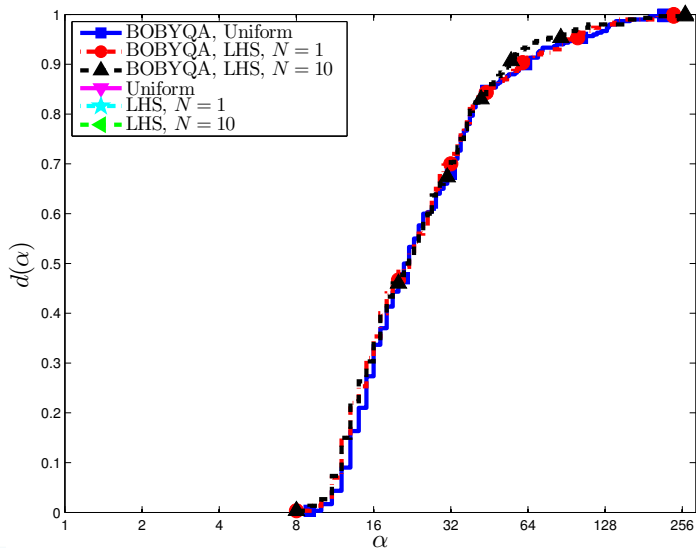
Data Profiles

$$f(x) - f_{(1)}^* \leq (1 - 10^{-4}) \left(f(x_0) - f_{(1)}^* \right)$$



Data Profiles

$$f(x) - f_{(1)}^* \leq (1 - 10^{-5}) \left(f(x_0) - f_{(1)}^* \right)$$



Closing Remarks

- ▶ Concurrent function evaluations can locate multiple minima while efficiently finding the global minimum.



Closing Remarks

- ▶ Concurrent function evaluations can locate multiple minima while efficiently finding the global minimum.
- ▶ Latin hypercube sampling appears to help find more minima in higher-dimensional problems.

Questions:

- ▶ Finding (or designing) the best local solver for our framework?
- ▶ Best way to process the queue?



Algorithm 3: AAML

Give each worker a point to evaluate

for $k = 1, 2, \dots$ **do**

 Receive from (longest waiting) worker w that has evaluated f

 Update \mathcal{H}_k and r_k

if *point evaluated by w is from an active run* **then**

if *Run is complete* **then**

 Update X_k^* , and mark points inactive

else

 Add the next point in its localopt run (not in \mathcal{H}_k) to Q_L

 Start run(s) at all point(s) satisfying (S1)–(S4), (L1)–(L6)

 Add the subsequent point (not in \mathcal{H}_k) from each run to Q_L

 Merge runs in Q_L with candidate minima within 2ν of each other

 Give w a point at which to evaluate f , either from Q_L or \mathcal{R}
